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UNIVERSITY OF COLORADO



NATIONAL BUREAU OF STANDARDS

SEMIANNUAL TECHNICAL STATUS REPORT

August 1971 through January 1972

Research Sponsored by
Advanced Research Projects Agency
ARPA Order No. 492

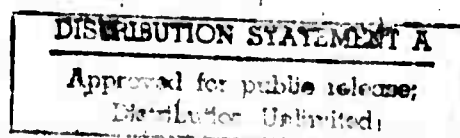


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March 1972

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REPORT



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I. Radiation Transfer and Charge Particle Transport in Gases

Project Coordinator: Dr. A. V. Phelps

Radiative Transfer (Drs. D. G. Hummer, J. Cassinelli, J. Castor, and

Mr. P. Kunasz)

Radiation hydrodynamics in spherical geometry. The case in which the gas does not significantly alter the radiation field, although the radiation field does modify the gas flow, is studied in detail. For a gravitating, spherically symmetric configuration of gas, the basic equations are

$$\frac{d}{dr} (\rho v r^2) = 0 \quad (1)$$

$$v \frac{dv}{dr} + \frac{GM}{r^2} + \frac{1}{\rho} \frac{dP_g}{dr} + \frac{1}{\rho} \frac{dP_R}{dr} = 0 \quad (2)$$

$$v \frac{d}{dr} (E_g) + v P_g \frac{d}{dr} \left(\frac{1}{\rho} \right) = 4\pi\sigma_1(J-B) , \quad (3)$$

expressing conservation of mass and momentum and the first law of thermodynamics for the gas, respectively, where ρ = density, v is velocity, P_g and P_R are the gas and radiation pressure and E_g is gas internal energy. Also, G = gravitational constant; M , the stellar mass, σ_1 , Stefans constant; κ , the true absorption coefficient. The momentum and energy equations involve moments of the radiation field. Convenient equations for these moments have recently been derived by Castor (unpublished) from the radiative transfer equation in a moving medium. These are

$$v \frac{d}{dr} \left(\frac{4\pi J}{c} \right) + \left(\frac{4\pi K}{c} \right) v \frac{d}{dr} \left(\frac{1}{\rho} \right) - \frac{4\pi v}{\rho c} \left(\frac{3K-J}{r} \right) = - \frac{1}{4\pi\rho r^2} \frac{dL}{dr} - 4\pi\kappa(J-B) \quad (4)$$

$$\frac{dK}{dr} + \frac{3K-J}{r} + \frac{v}{c} \frac{dH}{dr} - \frac{2v}{cr} H - \frac{2v}{c} \frac{1}{\rho} \frac{d\rho}{dr} H = -(\kappa + \sigma) \rho H \quad (5)$$

where J , H , and K are moments of the intensity, L is the luminosity and σ is the electron scattering coefficient. The flow is assumed to be radial and steady state, and in order to isolate the radiation - gas dynamics interactions, the run of mean intensity is prespecified to be that of freely streaming radiation, falling off as $1/r^2$. The radiative luminosity is approximately constant with r and is assumed identically constant in its effect on the radiative pressure gradient

$$\frac{1}{\rho} \frac{dP_R}{dr} = \frac{(\kappa + \sigma)\rho}{c} \frac{L}{4\pi r^2} \quad (6)$$

so

$$\Gamma = \frac{1}{\rho} \frac{dP_R}{dr} / \frac{GM}{r^2} \quad (7)$$

$$= \frac{(\kappa + \sigma)L}{4\pi c GM} = \text{const.} * (\kappa + \sigma) \quad (8)$$

The atmospheres are parameterized by the ratios 1) radiation pressure gradient/gravity, Γ and 2) absorptive opacity/electron scattering opacity, κ/σ . It is found that the ratio Γ must lie very close to unity in order for the sonic point r_c to lie reasonably close to the surface bounding the energy sources. The effective velocity of escape is related to the mean thermal velocity at the sonic point by $2.14 < [GM(1-\Gamma)/r_c] / (kT_c/m) \leq 3$. For a given value of Γ the behavior of the solutions for a large range of κ/σ is mapped. See Figures 1 and 2 showing the dependence of the velocity and temperature distribution on κ/σ , in these figures $x = r/r_{\text{sonic}}$. For $\kappa/\sigma > 10^{-5}$ the temperature distribution deviates negligibly from that in radiative equilibrium, i.e., $T^4 \propto J$. As κ/σ goes to smaller values the heating by the radiation field is less effective and the sonic point lies at increasingly large radii. This is illustrated in Figure 3, showing the

increase in gas energy with increasing radius. The calculation of the subsonic branch of the solution requires use of a two-point boundary value technique to satisfy the requirement that the solution approach the usual static behavior at the base of the atmosphere and be transonic farther out.

These solutions provide good initial trial-solutions for the more general problem involving radiative transfer coupled to the gas dynamics equation.

Radiative transport in a doublet. As a continuation of the study of radiative transport phenomena of interest in laboratory situations, we have analyzed in detail the case in which the upper state of the transition in question is an atomic doublet. The two levels of the doublet are collisionally coupled. The gas is assumed to be confined between two parallel walls and is illuminated in the wavelengths of the two lines by a radiation field with a prescribed wavelength dependence. At present non-radiative transport is not taken into account, and the emission and absorption coefficients are assumed to have a common frequency dependence, which is specified in advance. By the use of a generalized discrete ordinate method, the distribution of excited atoms in the two levels of the doublet are calculated, as well as the emergent radiation field.

The code has been checked extensively and is now ready for use. This calculation should be useful in determining the rate at which collisions mix the levels of the doublet.

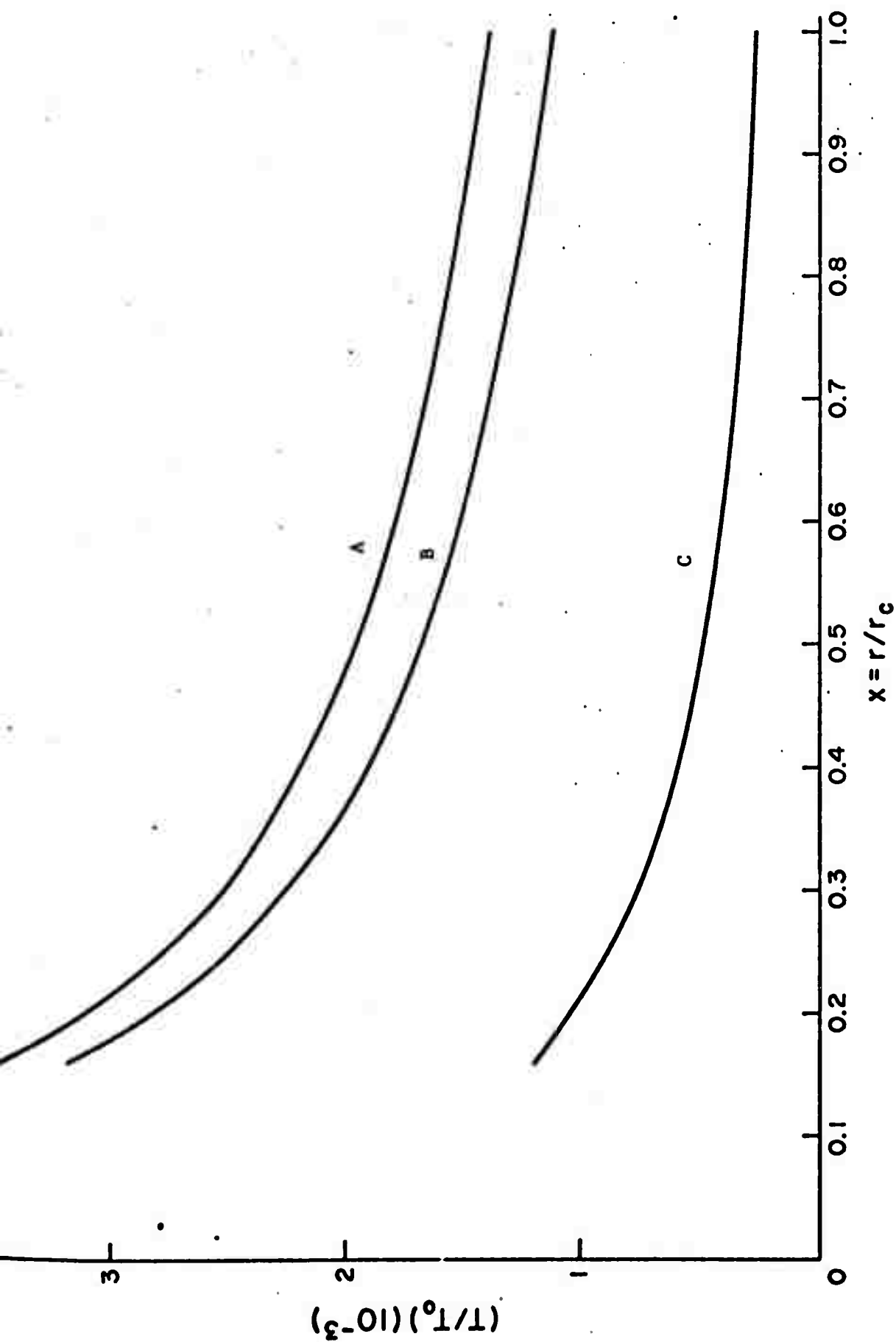


FIGURE 1 Temperature vs. x .

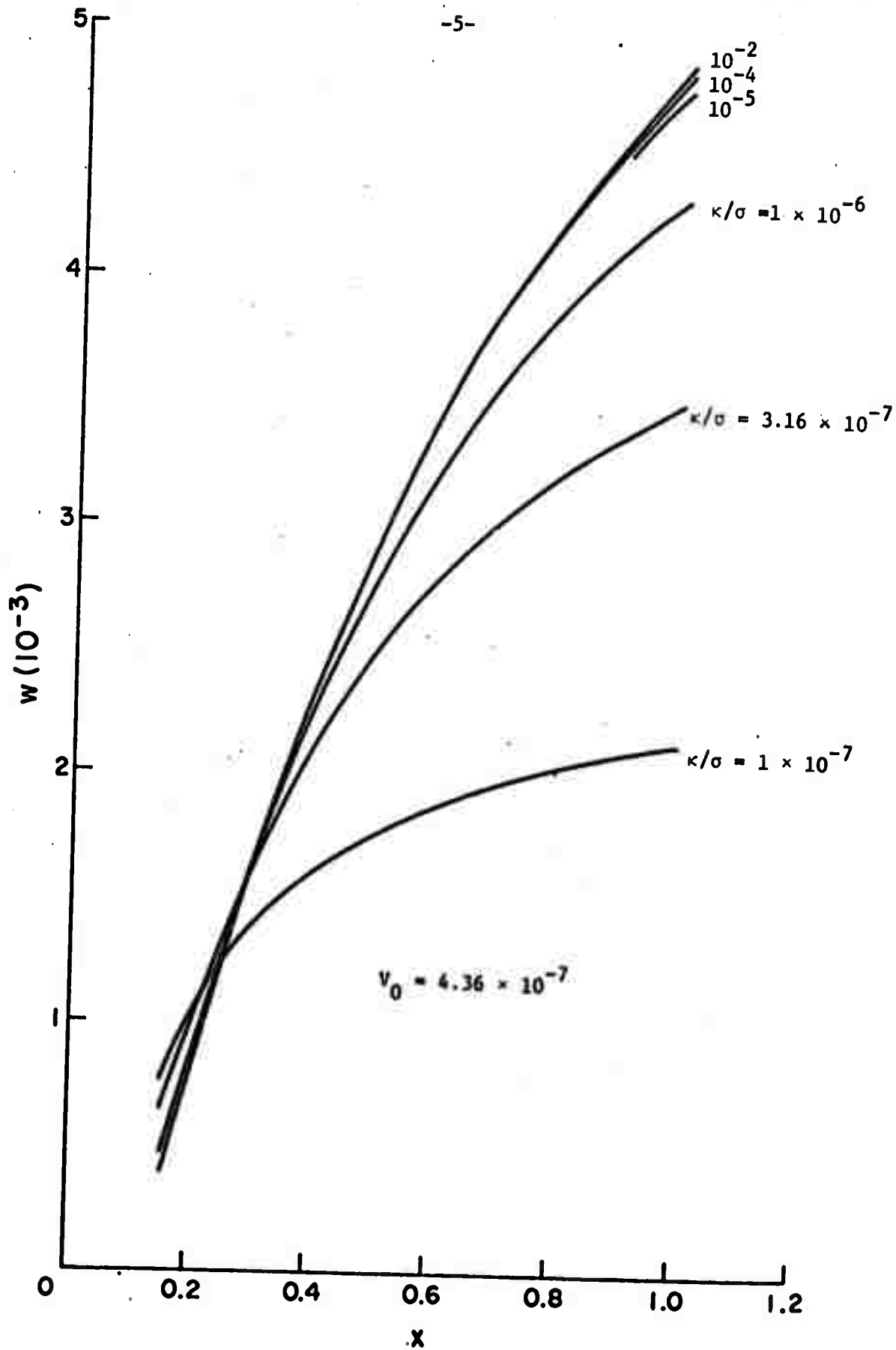


FIGURE 2

Velocity vs. x

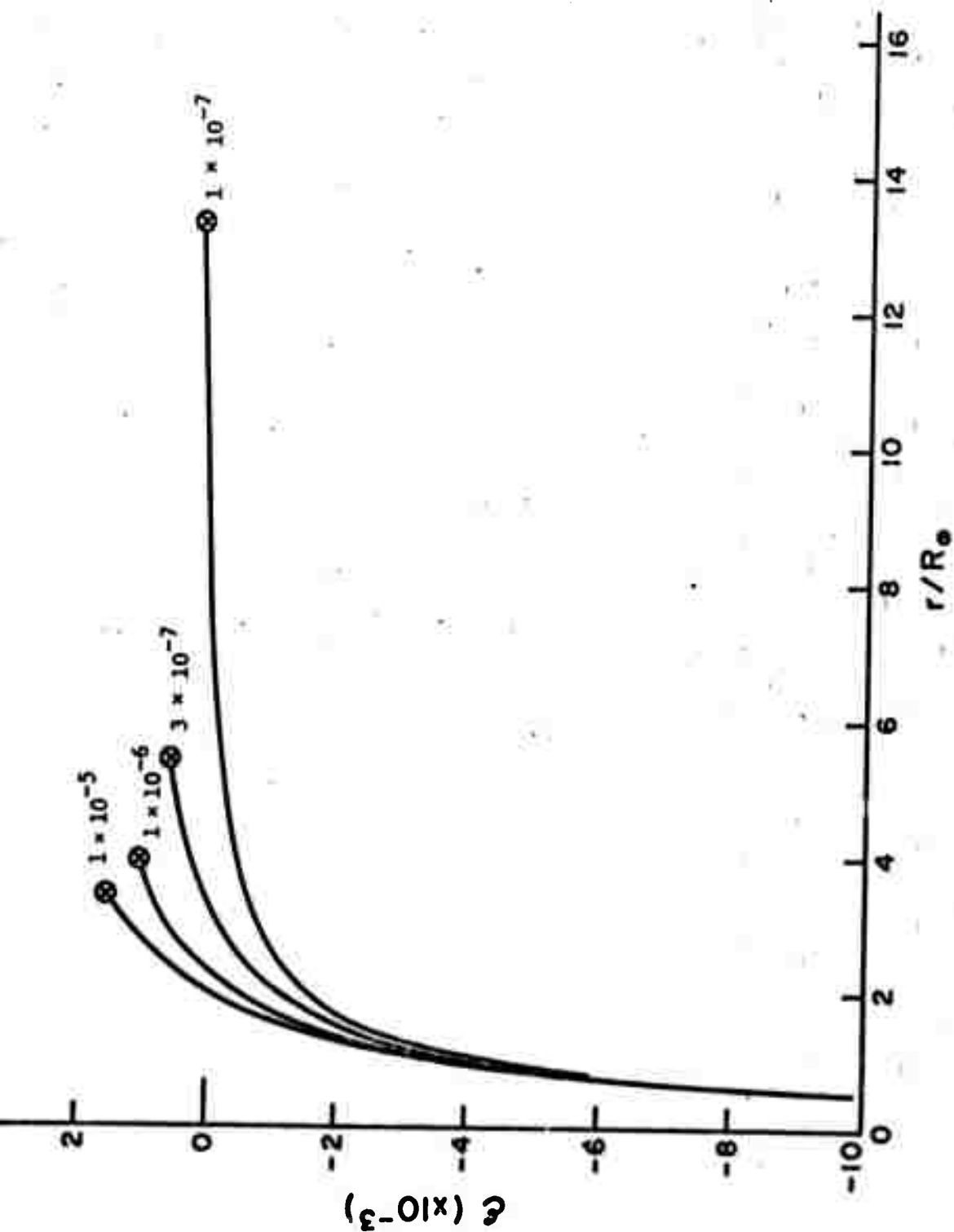


FIGURE 3

Energy vs. radius for various κ/σ . $\epsilon = \frac{v^2}{2} + \frac{5}{2} RT - \frac{GM}{r}(1-\gamma)$; \otimes marks the sonic point.

Scattering and Transport of Resonance Radiation (Drs. A. V. Phelps and J. Jenkins)

During the period of this report we have continued our experimental program designed to accurately determine the line profiles of the first resonance doublet of potassium at the moderately high densities, i.e., 10^{14} to 10^{16} atom/cm³, characteristic of our planned scattering and fluorescence measurements. The line profiles are obtained by computer analyses of measured absorption profiles so as to correct for the effect of the instrument profile of the monochromator. In the wavelength range between 0.4 and 10 Å from line center the corrected line profiles are found to be proportional to $(\Delta\lambda)^{-2}$ as expected for a dominant dipole-dipole interaction between the atom excited to the resonance state and a ground state atom. The line broadening parameters, i.e., the frequency full width at half maximum divided by the nominal atom density, determined for the wings of the line in these measurements are in good agreement with the values measured near line center by Lewis, Rebbeck and Vaughan.^{1*} Figure 4 shows a comparison of our measured absorption profile for the 7665 Å line with that predicted using the line center data and our measured instrument profile. Because of the presence of a relatively large density of rubidium, roughly 5%, in the nominally 99.999% pure potassium, we plan to make measurements of the product of the atom density and the oscillator strength using the specular reflection technique. Using known oscillator strengths for the resonance transitions we can determine the potassium density.

*References are listed at the end of each section.

Apparatus is being ordered for the cw laser scattering measurements of the redistribution in frequency which occurs upon reradiation of absorbed photons.

1. E. L. Lewis, M. M. Rebbeck and J. M. Vaughn, J. Phys. B: Atom. Molec. Phys. 4, 741 (1971).

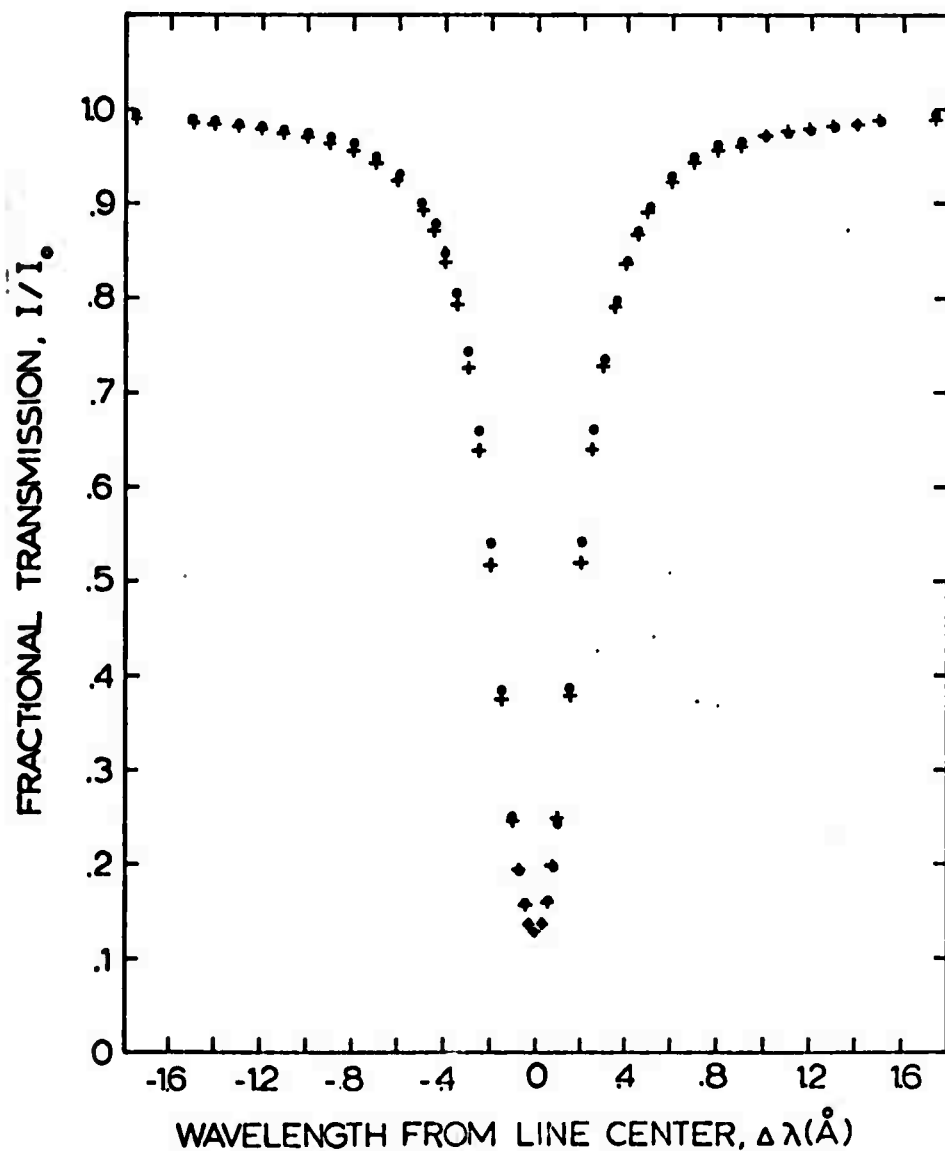


FIGURE 4

Comparison of the measured and theoretical fractional transmission profile of the potassium D₂ line ($\lambda = 7665\text{\AA}$) at a potassium density of $2.9 \times 10^{14} \text{ cm}^{-3}$. • Measured profile + Calculated profile

Plasma Spectroscopy (Dr. J. Cooper)

The results obtained with the parallel-plate accelerator for Stark broadening of Ar II and Ca II lines by electrons have now been published.¹ The Ca II data (although in agreement with theory) was in disagreement with most other experimenters (except one by a French group at a different temperature); however, recent results by H. Griem and coworkers (to be published) have confirmed our results:

The C-strap theta-pinch continuum light source is now providing a very satisfactory continuum,² and we have recently established that it is feasible to do absorption spectroscopy on ionized species.³ Preliminary results of spectra of C II and Si II have been obtained.

Tables of hydrogen line profiles⁴ using the unified theory are now complete. Theoretical profiles are in excellent agreement with recent experiments of Wiese, Kelleher, and Pagueke of NBS Washington (to be published). Major differences with previous calculations, even in the regime where the impact approximation is valid, have been traced to a mistake which recurred in the other work (see Ref. 4 for details).

Theoretical work on neutral atom broadening is continuing, with special emphasis being placed on the use of realistic potentials and the inclusion of m-mixing. A consistent formulation of the redistribution of radiation in the presence of collisions has been obtained in the impact regime.⁵ This work clarifies the role of the lower state, and the differences between elastic and inelastic collisions. Polarization effects and magnetic fields are also included.

1. J. S. Hildum and J. Cooper, Phys. Letters 36A, 153 (1971).
2. J. S. Hildum and J. Cooper, Rev. Sci. Instr. (in press).
3. J. S. Hildum and J. Cooper, JQSRT (in press).
4. C. R. Vidal, J. Cooper and E. W. Smith, Ap. J. Suppl. (to be published).
5. A. Omont, J. Cooper and E. W. Smith, Ap. J. (in press).

Stability of Discharges in Weakly Ionized Gases (Drs. L. Oster and

A. V. Phelps)

The objective of this theoretical project is to investigate quantitatively the factors which control the growth of instabilities in weakly ionized gas discharges, such as used in high power molecular lasers. In particular, we are developing theories applicable to the thermal instabilities which result in a decrease in gas density and a consequent increase in the rate of power input and of ionization. The importance of such considerations has recently been emphasized by Basov et al.¹ Our efforts during this report period have been limited to a more careful formulation of the theory. We expect to be able to begin numerical calculation soon after the beginning of the new contract period in July.

1. N. G. Basov et al., JETP Letters 14, 285 (1971).

Plasma Statistics (Drs. W. E. Brittin and W. R. Chappell)

Dr. Chappell has continued in his studies of the interaction of radiation and matter. At present he is working with a graduate student on the problem of Dicke narrowing of cyclotron radiation from plasmas. The hope is that such an effect, if observed, could be used to test various collision models for plasmas and give another way to measure diffusion constants. A paper with R. H. Williams "Microscopic Theory of Conductivity of a Weakly Ionized Plasma" has been accepted for publication in Physics of Fluids. Dr. Chappell gave a talk on this work at the Division of Plasma Physics Meeting in Madison in November. He also gave a talk on "Kinetic Theory of Partially Ionized Gases" at the A.P.S. Meeting in San Francisco in January.

Dr. Brittin is continuing with his work on a theory of composite particles. He has made some significant advances in developing a theory which correctly includes the proper symmetries of the atoms.

II. Ionization Kinetics and Reaction Rates

Project Coordinator: Dr. W. C. Lineberger

Ionization Kinetics (Dr. W. C. Lineberger, Mr. R. A. Beyer and
Mr. T. A. Patterson)

During the last six months our major emphasis has been placed on studies of negative ions of noble metals and the interpretation of near-threshold photodetachment data in terms of the electron-atom final state interactions. We have been greatly aided by the addition of Dr. Harmut Hotop to our group as a Postdoctoral Research Associate. Dr. Hotop, a gifted experimental physicist from the Physikalisches Institut der Universität Freiburg, receives his support from the German National Science Foundation.

Our standard arc negative ion source has proven to provide a copious current (~ 100 nA) of Se^- when seeded with a small quantity of SeO_2 . Figure 5 shows our photodetachment data for Se^- . From these data one can determine $\text{EA}(\text{Se}) = 2.0201 \pm .0003$ eV, and that the $^2\text{P}_{1/2} - ^2\text{P}_{3/2}$ fine structure splitting in the negative ion is 2279 ± 2 cm^{-1} . These values represent the first accurate measurements of this system and, by comparison with isoelectronic extrapolations, indicate that one can predict electron affinities and term splittings of Column VI atoms relatively well. A detailed study of the $\text{Se}^-(^2\text{P}_{3/2}) \rightarrow \text{Se}(^3\text{P}_2) + e(k)$ threshold shows deviations from the $\sigma \propto k$ threshold energy dependence at 5 millivolts above threshold. Here k is the momentum of the ejected electron. These deviations from the Wigner threshold law can be explained on the basis of an extension¹ of

O'Malley's treatment² of long range forces in the photodetachment process. Thus we obtain the following expression for the near threshold photodetachment of a bound p electron.

$$\sigma \sim kv \left[1 + \frac{4}{3} \alpha k^2 \ln 1.23\sqrt{\alpha} k + \left(\frac{2\pi\sqrt{\alpha}}{3} A - A^2 + A r_{p0} \right) k^2 - \frac{4\pi}{3} \alpha A k^3 \right]$$

where α is the polarizability of the atom, v is the frequency of the light, A is the scattering length characterizing the interaction of an s wave electron with the 3P_2 Se atom, and r_{p0} is an effective range parameter assumed to be smaller than A . A least-squares fit of our data to this formula yields a value for A of -5.8 ± 1 atomic units, and indicates that it is possible to obtain elastic scattering cross sections from threshold photodetachment data. We hope to apply these techniques to O^- , in order to obtain an independent estimate of the low energy elastic scattering cross section for electrons on atomic oxygen. These latter data are needed for a better estimate of the radiation emitted by an oxygen plasma.

We have developed a very simple source of metallic negative ions based upon the sputtering process. We have already obtained 10 mA beams of Au^- , Ag^- and Pt^- , and, based upon an analysis of the source performance, we should be able to obtain nanoampere negative ion beams of any metal whose electron affinity exceeds 30 meV. Figure 6 shows the Au^- photodetachment cross section together with the relevant energy levels. These data represent the first high resolution observation of photodetachment of a bound s electron, and demonstrate the validity of the Wigner threshold

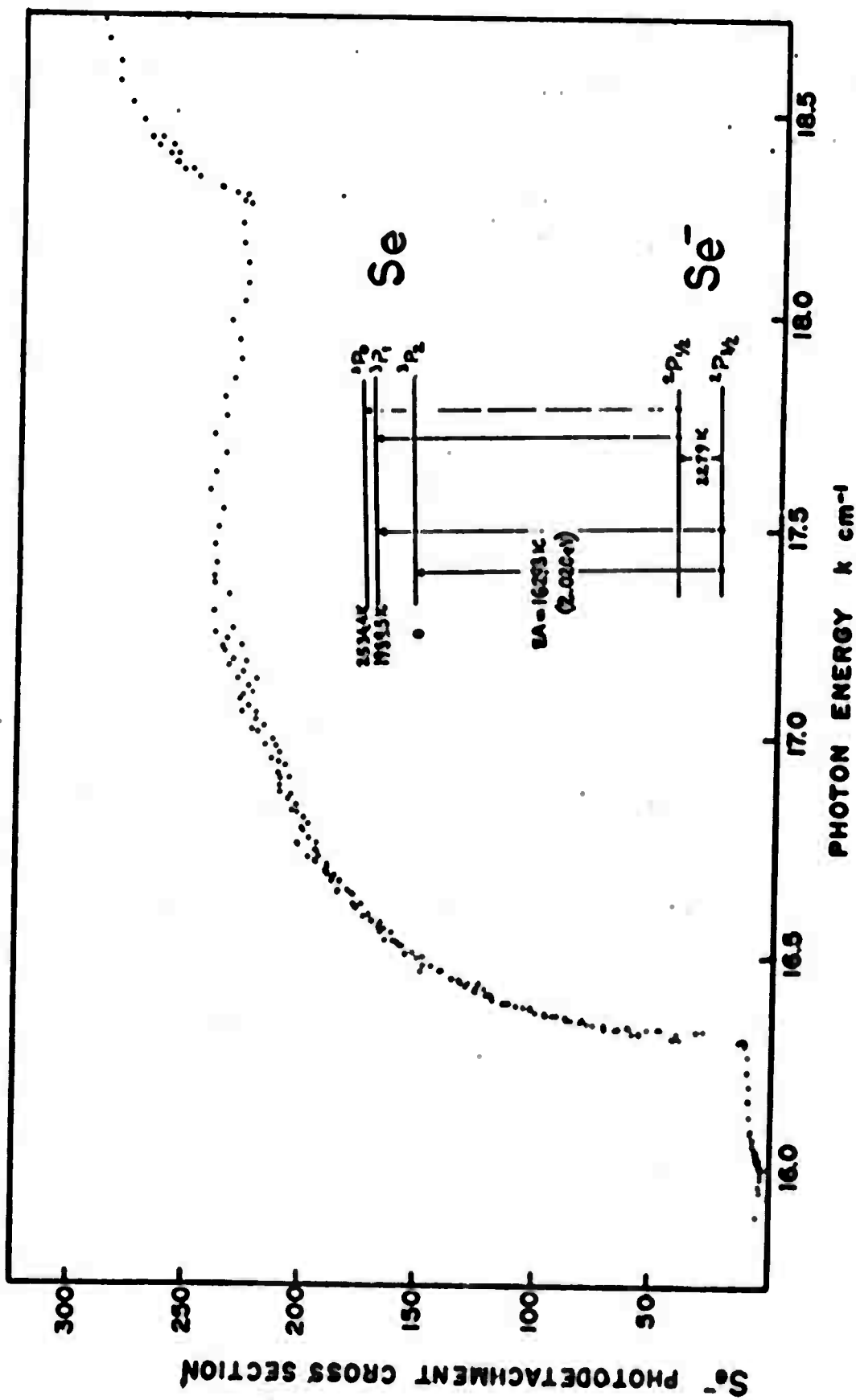


FIGURE 5

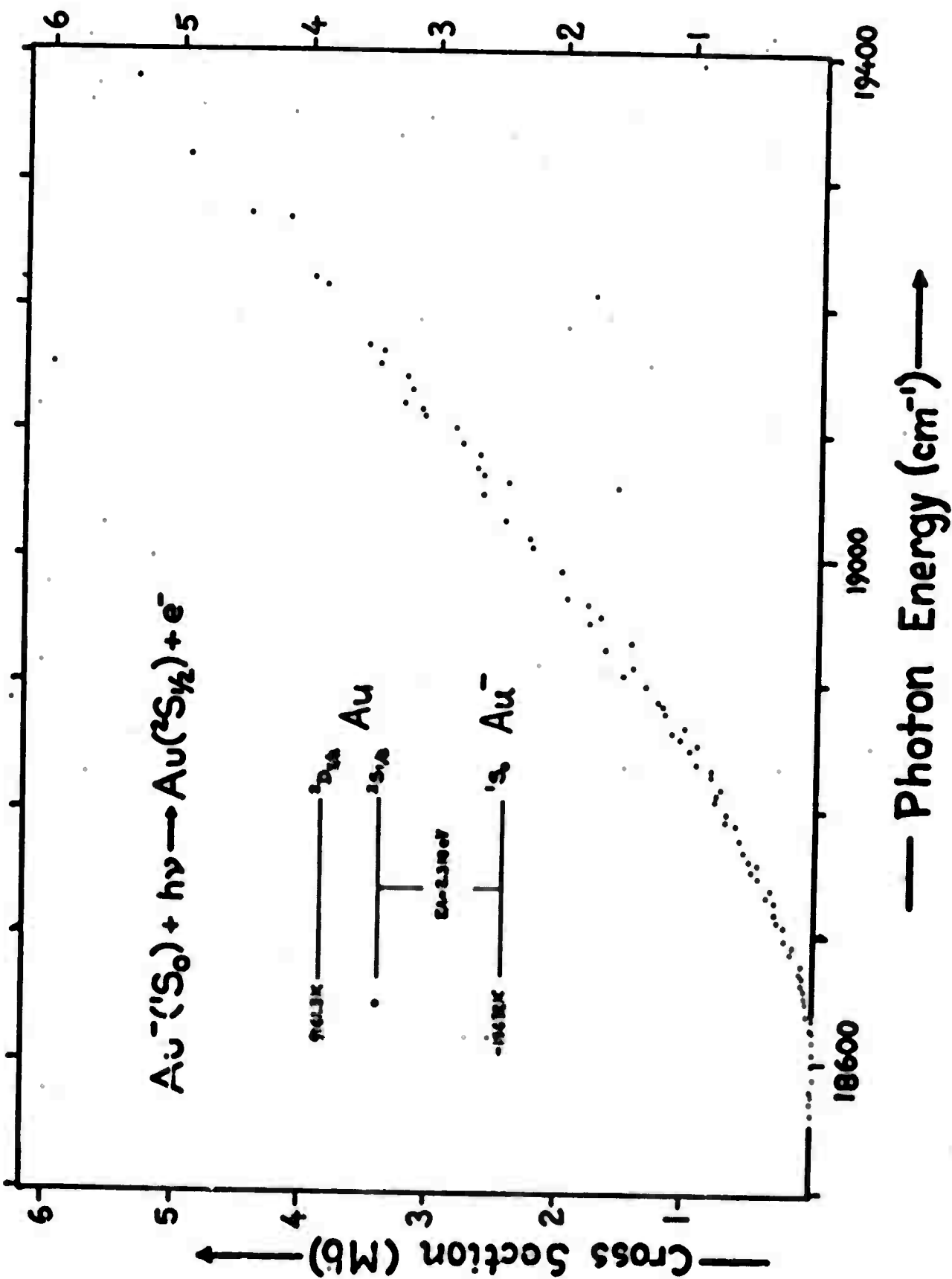


FIGURE 6

law for this case. In addition we find $EA(Au) = 2.310 \pm .001$ eV, which should be compared with an extrapolated electron affinity³ of $2.8 \pm .1$ eV. From these and other preliminary measurements on Pt^- and Ag^- , it is clear the extrapolation techniques, which work well for the Column VI atoms are in serious error for all transition metals. These studies of metal ions will be continued and extended in the next reporting period.

1. H. Hotop, T. A. Patterson and W. C. Lineberger (to be published).
2. T. F. O'Malley, Phys. Rev. 137, A1668 (1965).
3. R. J. Zollweg, J. Chem. Phys. 50, 4251 (1969).

JILA Information Analysis Center (Dr. L. J. Kleffer)

A manuscript entitled "Bibliography of Ion-Molecule Reaction Rate Data" by George A. Simnott has been submitted for publication. It will appear as an NBS Special Publication available from the Superintendent of Documents. Publication of this bibliography ends our efforts in this area.

With the assistance of the JILA Information Analysis Center a Workshop on Dissociation of Simple Molecules is being planned for March 16 and 17, 1972. Speakers and program have been arranged.

A project to critically review the information on the energy levels, and cross sections for populating them by electron impact, for molecular oxygen was initiated by Dr. Morris Krauss, NBS Washington. Dr. L. J. Kleffer NBS/JILA and R. D. Hudson NASA are participating in this review.

Assistance was given to Dr. A. V. Phelps in his attempt to obtain a "best set" of N_2 cross sections for use in laser modeling and modeling of other devices involving low pressure ionized gases. Data have been compiled and compared where possible. Data sets will now be used to predict the values of electron rate coefficients as deduced from swarm experiments. A best data set will be chosen on the basis of knowledge of the reliability and accuracy of the basic cross section data and their ability to predict the "correct" values of rate coefficient as deduced from electron swarm data.

An extensive compilation of electron swarm data and a complete bibliography of these data by J. Dutton is still being prepared. It is expected this manuscript will be submitted for publication during the next reporting period. It will be published in the Journal of Physical and Chemical Reference Data.

Molecular Dissociation Processes (Dr. L. J. Kieffer)

This project has temporarily been suspended due to the lack of a research assistant or postdoctoral personnel. During the next six months it is expected that additional data on dissociative ionization and pair formation of O_2 will be taken and the results written up for publication. Preliminary results for these two processes were discussed in the last semiannual report.

Electron Transport and Ionization Coefficients (Drs. G. E. Chamberlain,

L. J. Kieffer and A. V. Phelps)

This is a new project initiated in response to the need for more reliable electron transport coefficient and electron excitation and ionization rate coefficients. Such coefficients are essential for the prediction of the performance of gas discharge devices and systems, such as electron beam sustained lasers. Our first task is the determination of a complete set of rotational, vibrational and electronic excitation cross sections for low energy electrons in N_2 . Nitrogen is a major constituent in many high power lasers and in the atmosphere. New experimental data regarding electron excitation of rotational and electronic states have become available since the first attempt to obtain such a set of cross sections under the supervision of one of us (AVP) about 10 years ago. Our objective is to revise the cross sections for electrons in N_2 so as to be as consistent as possible with these new data while requiring consistency with electron transport data appropriate to electrical discharges. The calculations carried out thus far show that when the new excitation cross sections are used there are small but significant discrepancies between experimental and calculated ionization rate coefficients. We are currently reexamining the accuracy of the measured ionization coefficient data.

As a result of inquiries from various laser development groups we have carried out a short reevaluation of electron transport coefficient and attachment cross section data in NO . We note that according to the only

available data, obtained prior to 1930, the rate of electron energy loss in HCl for electrons of about 0.5 eV is much larger than for any other gas studied. If these data are correct it suggests that vibrational excitation cross sections in HCl are very large. This means that HCl might be useful in electric discharge lasers provided one can overcome the loss of electrons and HCl molecules by dissociative attachment.

III. Electron Energy Losses and Atomic Interaction Theory

Project Coordinator: Dr. E. C. Beaty

Theoretical Atomic Physics (Drs. D. G. Hummer and J. Castor)

Multichannel quantum defect theory. The quantum defect theory connects the problem of scattering of electrons by positive ions with the properties of the bound states of the same system. In the simplest cases it may be used to calculate partial elastic scattering cross sections given spectroscopic data for the bound states. In more complicated systems it provides a means of using theoretical scattering calculations to estimate the energies of and obtain approximate wave functions for excited bound states, so that one can compute oscillator strengths and photoionization cross sections for such states.

In the present investigation a combination of theoretical calculations and experimental data was used to obtain the electron scattering as a function of energy for the system $C^{+3} + e$. The ion C^{+3} has two low-lying terms, 2s and 2p, separated by 0.6 Ryd and the next lowest term 2.4 Ryd above. All observed terms of C^{+2} are derived from those two lowest terms of C^{+3} and only these terms were taken into account. For the S states and the three channel cases up to $L = 5$, as well as for the two channel cases up to $L = 3$, the scattering problem has been solved using the integro-differential equation method at energies above the 2p threshold. These results have been supplemented with other calculations using the distorted wave method for all cases up to $L = 9$.

The present work has produced an essentially complete term diagram of C III up to $L = 5$, including the autoionizing states with their rates of autoionization as well. The configuration mixing coefficients are a by-product

of this calculation, and they are now available for future use in Quantum Defect Method calculations of the oscillator strengths and the photo-ionization cross sections for excited states.

Electron-Excitation Cross Sections. These calculations have been completed for all transitions among the first eleven terms of N III and the first five terms of N IV (this calculation is preliminary to one involving nineteen terms). Configuration interaction bound state wave functions including six configurations ($2s^2 2p$, $2s 2p^2$, $2p^3$, $2s^2 3s$, $2p^3$, $2s^2 3p$, $2s^2 3d$) for N III and three configurations for N IV ($2s^2$, $2s 2p$, $2p^2$) for N IV. The corresponding terms are given in Table 1. Scaled statistical model radial wave functions were used¹ and the scattering calculation was performed using the unitarized Distorted-Wave Approximation. The collision strength Ω_{ij} for each transition was obtained at six energies, from which the de-excitation rate constant [$E_i > E_j$],

$$q_{i \rightarrow j}(T_e) = \frac{8.63 \times 10^{-6}}{\omega_i T_e^{1/2}} \int_0^\infty \Omega_{ij}(k_1^2 = W + E_i - E_j) e^{-W/kT_e} d\left(\frac{W}{kT_e}\right)$$

was evaluated using a highly efficient and accurate spline-interpolation technique. The result for $10^3 \leq T_e \leq 10^5$ is written in the form

$$q_{i \rightarrow j}(T_e) = T_e^{-1/2} P(x), \quad x = \log_{10}(10^{-4} T_e)$$

where $P(x)$ is a low order polynomial. The corresponding excitation rate constants are easily obtained from the familiar detailed balance relation. Electric dipole and quadrupole absorption oscillator strengths obtained from the bound state functions appear in Table 2. If better oscillator strengths

become available for the dipole transitions, the collision rate constants for the corresponding transitions should be scaled by the ratio of the new values to those tabulated in Table 2.

1. W. Eissner and H. Nussbaumer, J. Phys. B: Atom. Molec. Phys. 2, 1028 (1969).

TABLE 1

<u>Level #</u>	<u>N III</u>	<u>N IV</u>
1	$2s^2 2p^2$	$2s^2 1s$
2	$2s 2p^2$	$2s 2p^3$
3	$2d$	$1p^0$
4	$2s$	$2p^2 3p$
5	$2p$	$1d$
6	$2p^3$	$1s$
7	$2d^0$	
8	$2s^2 3s$	$2s$
9	$2p^3$	$2p^0$
10	$2s^2 3p$	$2p^0$
11	$2s^2 3d$	$2d$

TABLE 2

<u>Transition</u>	<u>f (e1)</u>	<u>10⁶ f (e2)</u>
N III		
1-3	.133	
1-4	.102	
1-5	.44	
1-7		.960
1-8	.0280	
1-9		.182
1-10		6.64
1-11	.453	
2-7	.171	
3-4		.0139
3-7	.208	
3-8		.333
3-9	.144	
3-10	.00349	
3-11		.632
4-9	.200	
4-10		.0179
4-11		2.60
5-7	.179	
5-9	.265	
5-10	.00495	
7-9		.0341
7-10		.00107
7-11	.00078	
8-9	.00065	
8-10	.81869	
8-11		8.80
9-11	.00020	
10-11	.443	

N IV

1-3	.634	
1-5		1.14
2-4	.248	
3-5	.213	
3-6	.164	
5-6		.0468

Atomic Interaction Theory (Drs. S. Geltman and D. W. Norcross)

Coulomb-projected Born approximation. The application of this approximation to the 2^1S and 2^1P excitation of helium by fast electrons has been completed.¹ The results are in fair absolute agreement with the experimental findings of Opal and Beaty, and orders of magnitude better than the usual Born approximation at large angle scattering (Fig. 7). The remaining discrepancy between the present theory and experiment is probably due to inaccuracies in our atomic wave functions and the fact that 200 eV is still too low an energy (the theory is expected to be valid at higher energies). The limiting high energy dependence for all non-forward angles is again found to be E^{-3} , as was the case for hydrogen atom excitation. This is in marked contrast to the Born values of E^{-6} and E^{-7} (for $s \rightarrow s$ and $s \rightarrow p$ excitations, respectively). A simple physical interpretation of the E^{-3} dependence is obtainable by regarding $\frac{d\sigma_{if}}{d\Omega}$ to be the product of the Rutherford differential cross section for the elastic scattering of the electron by the nucleus ($\sim E^{-2}$) and the semi-classical probability for excitation by an electron on this Coulomb trajectory ($\sim E^{-1}$).

We are now attempting to apply the present approximation to the ionization of hydrogen by electron impact. The integrals involved become much more complicated than in the excitation case and more numerical integration is necessary. The quantity of interest is the triply differential cross section $d^3\sigma/d\Omega d\Omega_e dE_e$, where $d\Omega$ and $d\Omega_e$ are the elements of solid angle for the scattered and ejected electrons and dE_e is the element of energy of the ejected electron. Generally Ω and E_e are held fixed and the resulting $d^3\sigma$ is depicted in a polar plot as a function of θ_e . A comparison of theory and experiment for this quantity is a much more sensitive test than is the total ionization cross section.

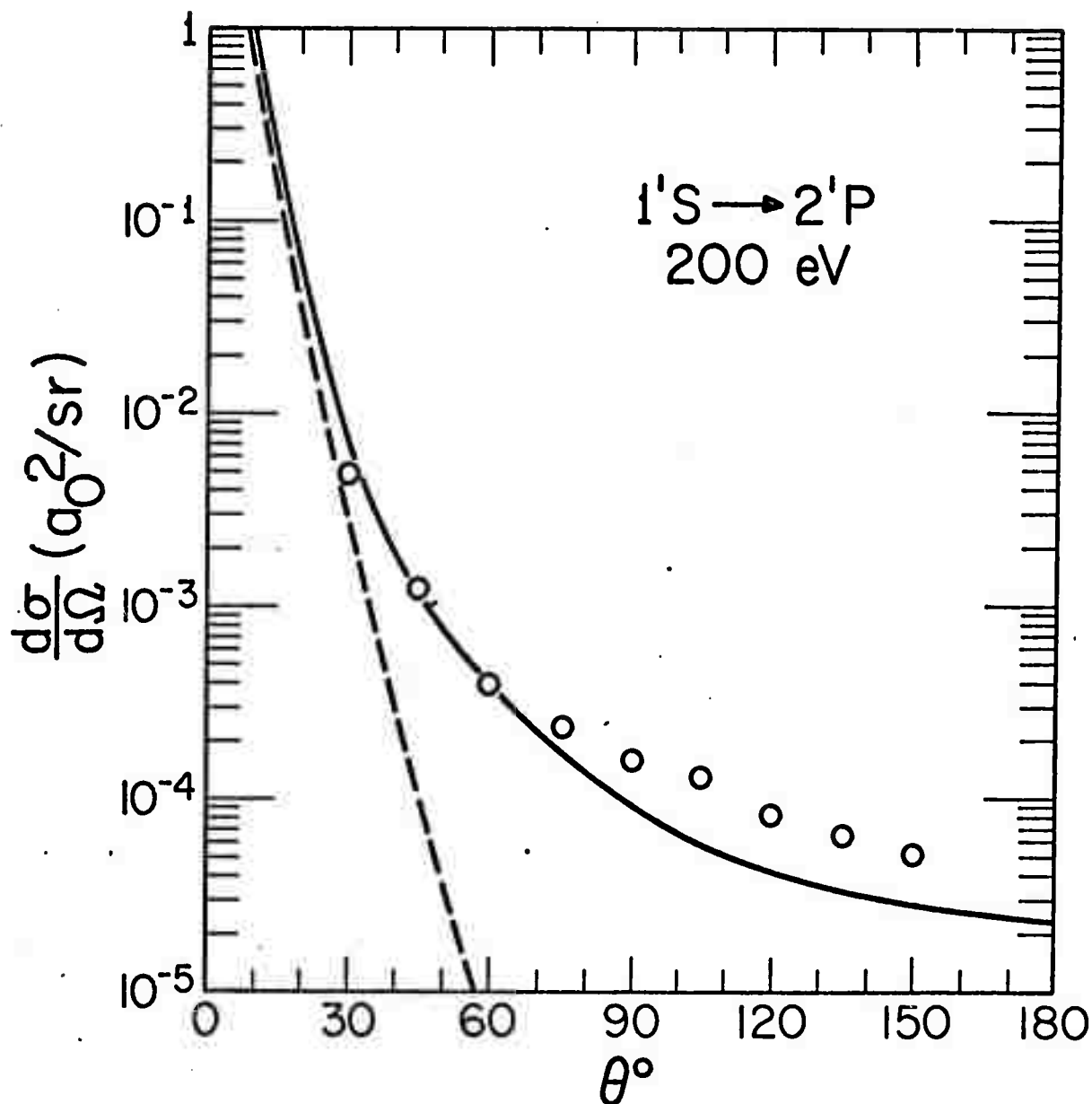


FIGURE 7

Differential cross section for $1^1S \rightarrow 2^1P$ transition at 200 eV.

Present approximation (solid curve), Born approximation

(dashed curve), and experiment (open circles--Opal and Beatty).

Electron scattering and photoionization. Calculations of low energy elastic scattering² for Na have been extended up to 5 eV incident electron energy and have been performed in both the two- and four-state close-coupling approximations, with results in excellent agreement with recent experiments.^{3,4} These results also indicate that the previously reported disagreement with experiment at low energies cannot be attributed to lack of convergence in the calculations, the two- and four-state results being nearly identical at low energies. A similar four-state calculation for Li is contemplated, as there remains a serious disagreement between previous two-state calculations⁵ and experiment.⁶ The IMPACT code of Prof. M. J. Seaton, rather than the present program will be used, at a considerable saving in computer time.

As an aid to studies of electron scattering by the heavier, one electron systems the target models are being tested by comparison of calculated and available experimental photoionization cross sections. These are, in principle, relatively simple calculations, and the cross sections are themselves of intrinsic interest. These cross sections are known to be strongly influenced by core polarization and the spin-orbit effect, particularly for cesium, which is currently being studied. Preliminary results have served to help discriminate between two conflicting experimental studies of the spin-orbit effect in cesium photoionization,^{7,8} and a report on this work has been readied for publication. A complete calculation of the photoionization cross section for cesium is underway. Preliminary results for

Mg^+ indicate that the core polarization effect is important for this species, for which no experimental results are available.

Having obtained reliable target models for calculations of electron scattering by Mg^+ , Ca^+ , and Ba^+ , the IMPACT code and the techniques discussed above will be used to compute the photoionization cross sections of Mg, Ca and Ba. Only the second of these is reliably known,⁹ and will serve as a useful check on the work.

1. M. B. Hidalgo and S. Geltman, J. Phys. B: Atom. Molec. Phys. (in press).
2. D. W. Norcross, J. Phys. B: Atom. Molec. Phys. 4, 1458 (1971).
3. E. Enemark and A. Gallagher (to be published).
4. D. Andriak, M. Eyb, and H. Hoffman, J. Phys. B: Atom. Molec. Phys. 5, L15 (1972).
5. E. M. Karule, J. Phys. B: Atom. Molec. Phys. 3, 860 (1970).
6. H. Haffner and H. Kleinpoppen, Z. Physik 198, 315 (1967).
7. U. Heinzmann, J. Kessler and J. Lorenz, Z. Physik 240, 42 (1970).
8. G. Baum, M. S. Lubell and W. Raith, Phys. Rev. Letters 25, 267 (1970).
9. V. L. Carter, R. D. Hudson and E. L. Breig, Phys. Rev. A 4, 821 (1971).

Electron Energy Losses (Drs. E. C. Beaty and J. Mauer)

Data on differential ionization cross sections have now been prepared for publication. Data on helium have been published in Phys. Rev. A¹ with a complete evaluation of reliability of experimental procedures. A complete tabulation of all the data has been prepared for publication in Atomic Data (previously available as JILA report 108).

Modifications of equipment are being made to permit reducing some of the uncertainties and an extension of these measurements. An additional stage of differential pumping is being added to permit a more highly collimated molecular beam. The electron gun support is being rebuilt to permit measurements at smaller angles. Also a second electron detector will be added to permit measurement of all the dynamic variables relevant to ionization.

1. W. K. Peterson, E. C. Beaty and C. B. Opal, Phys. Rev. A 5, 712 (1972).

IV. Electron-Atom Collisions

Project Coordinator: Dr. S. J. Smith

Electron-Ion Recombination (Drs. F. L. Walls and C. H. Dunn)

This experiment employs trapping of ions in a dc electric and magnetic field configuration to investigate collisions of these ions with other particles. In particular dissociative recombination of these ions with monoenergetic electrons will be investigated over an electron energy range from 0 to several eV.

Significant progress has been made during the reporting period. Ions have been trapped and non-destructively observed with good signal-to-noise. Figure 8 shows a scan of a trapped ion with mass 18. (The scan parameter is frequency. The peak occurs at the resonant frequency of mass X in the harmonic electrostatic well). Trapping lifetime has been shown to be greater than 5 hours, and the number of ions is about 10^4 .

Figure 9 demonstrates recombination of these ions with electrons. In Figure 9a an electron current of 1.2×10^{-9} Amp with about 0.5 eV energy bombarded the trapped ions starting at about 50 sec. In this plot the integral under the ion peak is shown as a function of time, and it is seen that ions disappear with a characteristic decay time after the electrons are introduced.

In Figure 9b electrons with 15 times higher energy (7.5 eV) are introduced with a correspondingly higher current (to keep space charge effects comparable), and we see that the recombination cross section is small enough at this energy that no depletion of ions is observed.

Using the technique to measure absolute cross sections requires knowledge of the density and spatial distribution of ions in the trap. To measure this, a Bendix Channeltron Bundle multiplier is being placed at one end of the trap, and the trap slightly "tilted" to that end. Ions will be resonated out of the trap onto the bundle. Ions impinging on the front surface of the multiplier will produce current pulses out the back whose position in the XY plane is the same as the parent ion. Using a resistive anode for the multiplier, and pulse height sorting, the radial distribution of the ions can be determined with a resolution of 0.006". During the report period this device has been assembled along with relevant electronics and an electron gun delivering a sharply focused beam to test the device.

Currently the instrument is being "cleaned up" prior to starting serious measurement. Improvements are being made to the pumping and gas handling systems, and some parts of the electronics are being improved and consolidated. Measurements are being planned on NO^+ , X_2^+ , O_2^+ , H_2O^+ , and ND^+ up to an electron energy of about 7 eV and with an energy resolution of 0.030 eV.

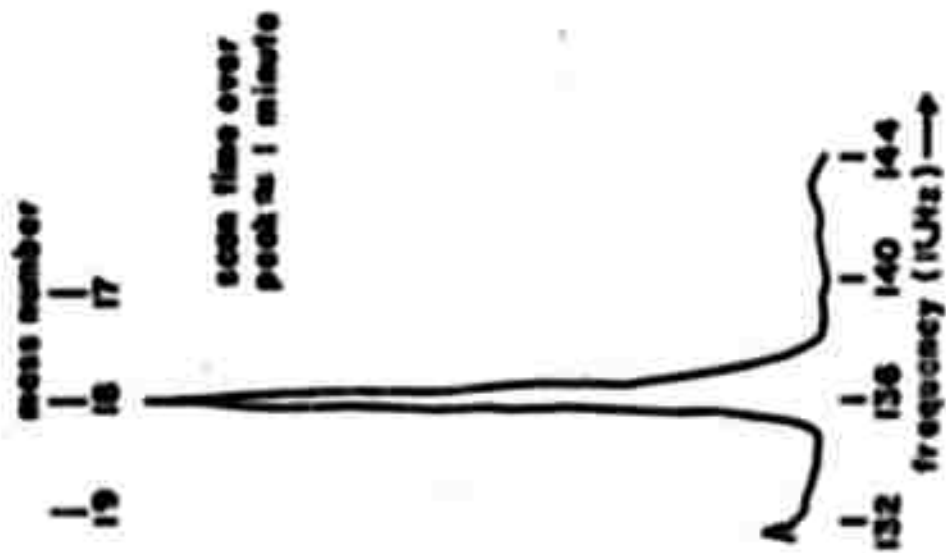


FIGURE 8

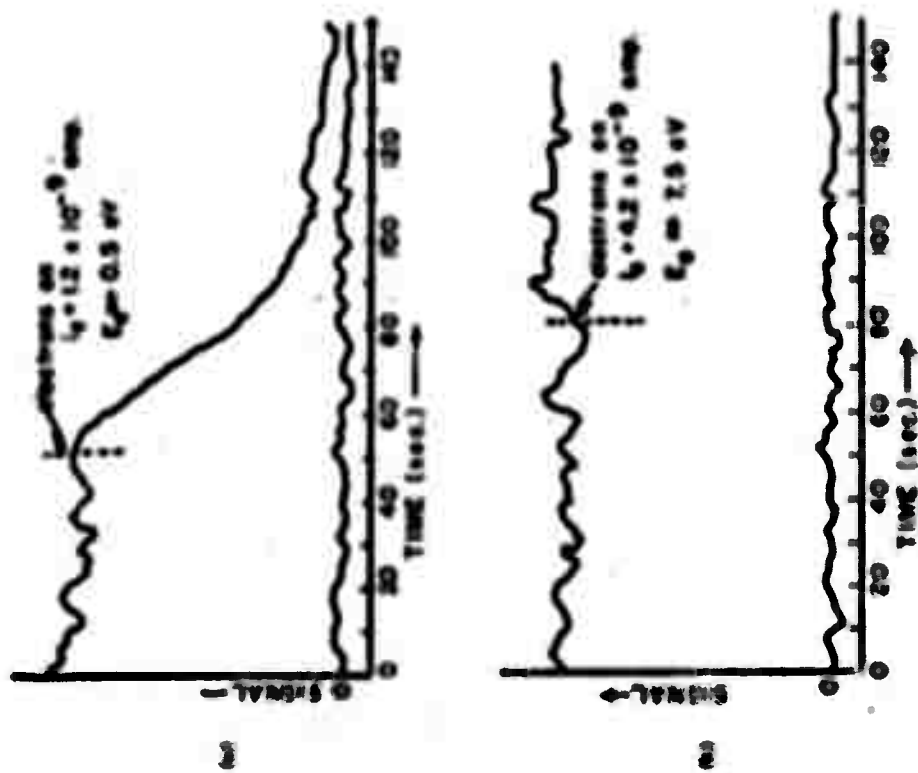


FIGURE 9

Excitation of Ions by Electron Impact (Drs. G. N. Dunn, D. Crandall, and Mr. P. O. Taylor).

This project is to measure the cross sections for electron-impact excitation of X_2^+ , Ca^+ , and Na^+ using crossed beams of variable energy electrons and the respective ions and observing the resultant resonance radiation along the third perpendicular direction. Preliminary results were reported earlier.

During the period covered by this report more precise data were accumulated for the excitation of Ca^+ . Absolute calibration was pursued further, and a serious problem was discovered with the copper point black body being used as a radiometric standard. This has led to a reassessment of the standards used, and currently a tungsten strip lamp has been installed for the purpose.

V. Radiation Processes

Project Coordinator: Dr. A. C. Gallagher

Collisional Radiation (Dr. A. C. Gallagher)

The interaction potentials for cesium interacting with the inert gases have been obtained from the studies of extreme-ultraviolet continuum radiation. The cesium-argon potentials are shown in Figure 10. A report of this work has been submitted for publication.

The experiment has now been interfaced with computer control and measurements of the rubidium-inert gas spectrum are proceeding.

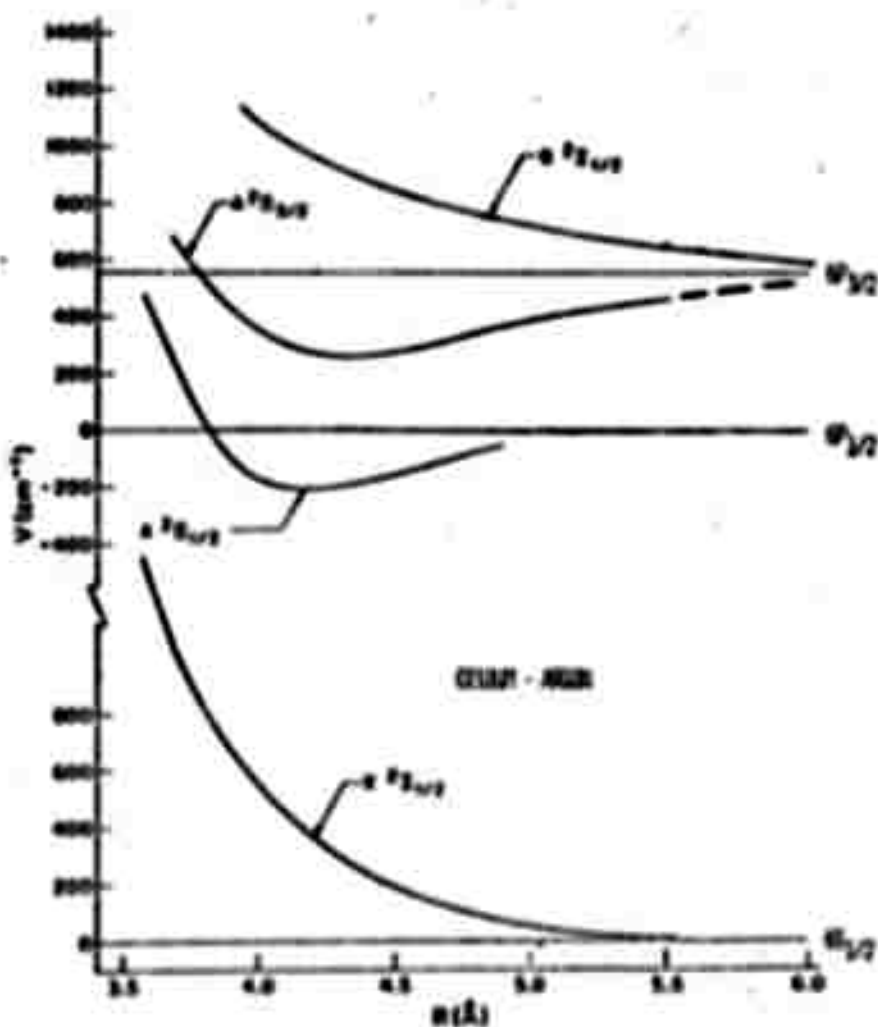


FIGURE 10

Negative Ion Studies (Dr. J. Hall and Mr. R. A. Bennett)

During this period the major effort has been invested in fine-tuning the apparatus and in getting good data for SO^- . As the uncertainties of the line center and line strengths data project directly into uncertainties in r_e and ω_e for the negative ion state, it was decided to try to improve the symmetry of the electron analyzer function. (The optimum analyzer potentials depend on the contact potentials of the surface, and quite possibly these have drifted over the last year or so since the previous adjustments.)

It proved possible simultaneously to improve the symmetry of the analyzer function as well as to improve the absolute counting rate and ratio of counting rates (laser on/laser off). Thus very good data for line center determination could be obtained. These data, after computer fitting, taken along with the angular distribution data previously obtained by Mr. Bennett, should allow complete determination of the properties r_e , ω_e and E_A for SO^- . An additional new facet of this work is the presence of an observable population of $v = 1$ negative ions, giving good confirmation of our ω_e value. The use of isotopic substitution to influence ω_e in a known way has given unique corroboration of our vibrational quantum number assignments. The SO^- problem is currently being finished by Mr. Bennett as his Ph.D thesis.

The NO^- and O_2^- papers were returned by the referee for Physical Review with some important and useful comments, particularly concerning the rotational correction. Dr. R. J. Celotta, although he has now left JILA, is collaborating on a still more refined calculation of the effect of finite rotational temperature on the observed vertical detachment energies.

When Mr. Bennett is completely finished with the experimental part of his work, we plan to adapt the new "sputtering" negative ion source, developed at JILA by Drs. W. C. Lineberger and H. Hotop, to our apparatus. We should be able to provide "survey quality" information, say ± 10 mV, for the negative ion states of Pt, Au, Ag, etc. Very possibly negative alkali beams will be available also from this kind of source.

Manuscripts Involving ARPA Funds

Listed below are papers submitted for publication during the period covered by this report. Co-authors not connected with JILA are shown in parentheses.

- R. J. Celotta, R. A. Bennett, J. L. Hall, M. W. Siegel and J. Levine, "Molecular photodetachment spectrometry II. The electron affinity of O_2 and the structure of O_2^- ," submitted to Phys. Rev. A.
- W. R. Chappell (and R. H. Williams), "Microscopic theory of a weakly ionized plasma," to appear in Phys. Fluids.
- S. Geltman, "Applications of pseudo state expansions," in VII ICPEAC Invited Talks and Progress Reports (T. R. Gowers and F. J. deHeer, Eds., North-Holland, Amsterdam, in press).
- M. B. Hidalgo and S. Geltman, "A high energy approximation III. Helium excitation by electrons," to appear in J. Phys. B: Atom. Molec. Phys.
- W. C. Lineberger and T. A. Patterson, "Two photon photodetachment spectroscopy. The $C_2 - 2\Sigma$ states," Chem. Phys. Letters 13, 40 (1972).
- C. B. Opal and E. C. Beaty, "Measurements of large angle inelastic cross sections in helium," to appear in J. Phys. B: Atom. Molec. Phys.
- C. B. Opal, E. C. Beaty and W. K. Peterson, "Tables of secondary-electron-production cross sections," to appear in Atomic Data.
- W. K. Peterson, E. C. Beaty and C. B. Opal, "Measurements of energy and angular distributions of secondary electrons produced in electron impact ionization of helium," Phys. Rev. A 5, 712 (1972).
- M. W. Siegel, R. J. Celotta, J. L. Hall, J. Levine and R. A. Bennett, "Molecular photodetachment spectrometry I. Affinity of nitric oxide and the molecular constants of NO^- ," submitted to Phys. Rev. A.